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NSR&D FY15 Final Report: Modeling Mechanical, Thermal, and Chemical Effects of Impact

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Abstract

The main goal of this project is to develop a computer model that explains and predicts coupled mechanical, thermal and chemical responses of HE under impact and friction insults. The modeling effort is based on the LANL-developed CartaBlanca code, which is implemented with the dual domain material point (DDMP) method to calculate complex and coupled thermal, chemical and mechanical effects among fluids, solids and the transitions between the states. In FY 15, we have implemented the TEPLA material model for metal and performed preliminary can penetration simulation and begun to link with experiment. Currently, we are working on implementing a shock to detonation transition (SDT) model (SURF) and JWL equation of state.

1 Introduction

Lagrangian finite element methods are the traditional choice to model solid deformations involving void growth and material failure. However, difficulties arise when the material experiences large deformation resulting in heavily skewed elements. To avoid this numerical difficulty, we use the dual domain material point (DDMP) method [1]. The DDMP method is an improved version of the material point method (MPM) [2], which is the particle-in-cell (PIC) method [3] reformulated using the concept of virtual work. The most significant difference between the material point methods and the FEM is that material point methods retain Lagrangian capabilities while using an Eulerian mesh, rather than a Lagrangian mesh as in FEM. The Lagrangian capability of the material point method relies on the Lagrangian particles, also called material points, that are free to move about the Eulerian mesh, and thus can be used to carry the history dependent quantities in ductile material models without the difficulties of numerical diffusion. Material point methods avoid mesh distortion difficulties associated with Lagrangian methods and numerical diffusion difficulties associated with Eulerian methods, because material point methods use both an Eulerian mesh and Lagrangian particles. The DDMP method is the latest version of the material point method with the numerical noises reduced and accuracy increased. It has been applied to many large deformation problems [4, 5] with success.

In this year we use the DDMP method as a tool to implement the TEPLA model [6, 7] and performed a continuum mechanics calculations to compared with Flyer plate experiments performed at Los Alamos National Laboratory [8]. The present work has three objectives. The first objective is to evaluate whether the DDMP method can represent the major physics involved in this problem, including plastic flow, porosity growth, material damage, and failure. The second objective is to understand the numerical properties of the DDMP method in modeling materials with ductile damage and strain softening. The third objective is to use the numerical capability of DDMP to evaluate the relative importance of different physical mechanisms and numerical treatments often used in modeling this impact and failure problem.

The basis for the flyer plate problem is straightforward: A plate is traveling at high velocity and strikes another stationary plate. These are referred to as the flyer plate and the target plate, respectively. The target plate has a thickness double that of the flyer plate. Upon impact, a compression shock travels through both plates to opposite surfaces, and the reflected tensile expansion fans collide at the center of the target plate, if the flyer and the target plates are made of the same material. This problem is physically well defined, while presenting numerous challenges for numerical techniques, including shock propagation, material softening and failure, and history dependence. Therefore we choose this problem to test the TEPLA implementation and the DDMP method. This work of implementing the TEPLA model and comparison of the DDMP results to flyer plate experiments has been submitted for publication [9]. In this report we only describe our major findings in the following section. Readers interested in details of the work are referred to the attached manuscript.

To demonstrate potential applications of the DDMP method and the TEPLA model, parallel to the TEPLA implementation effort, we have setup and performed a preliminary can penetration simulation and begun to link with experiment. The only difference in the model used in this calculation and the TEPLA model is the void growth part. The coupled mechanical and thermal response is considered in this calculation.

Furthermore, to consider the effect of HE response, we are implementing a shock to detonation transition (SDT) model, SURF, with the JWL equation of state. Currently, it works well for one-dimensional cases, and the results agree with experimental data.

The planned work for FY 16 is to use the TEPLA model in the "can" calculation, to complete the model implementation for HE response, and then to perform coupled mechanical, thermal, and chemical responses under impact.

2 TEPLA Implementation and Results

We have implemented the ductile damage and failure model of Addessio and Johnson as described in [6, 7]. Early implementations [6] used a constant plastic flow stress. Following [10], in the present work we use a Gurson surface to define deformation in the plastic regime. We also implemented the overstress model described by Addessio and Johnson [7], and Zuo and Rice [10]. A Hancock-Mackenzie formulation is used to describe material failure in terms of the plastic strain and porosity [11].

Shock-loaded metals have been modeled as highly viscous fluids [12] in which the energy dissipation is modeled as if the material were a Newtonian fluid. This method can be justified if the plastic deformation overwhelms the elastic deformation. Although for the cases considered in this work this condition is not satisfied, the concept of viscosity does bring in an interesting point. In traditional plasticity models for metals, the compressibility of the material is usually neglected, while a bulk volumetric deformation is allowed in [6, 7, 10] and in the present work. To consider the energy dissipation associated with the volumetric deformation, we explore the effect of the bulk viscosity.

In fact we have also experimented adding a shear viscosity to the equation. Similar to the finding reported in [5], we find that shear viscosity effects are negligible because the energy associated with deviatoric deformation has been sufficiently dissipated by the plastic flow. However, the bulk viscosity remains important as shown by the numerical examples. This is because that energy dissipation associated with the volumetric deformation is not considered elsewhere in this model.

Flyer plate experiments performed at Los Alamos National Laboratory [8] used metal plates of pure tantalum, with an initial flyer plate velocity of 249 m/s. The experimental and numerical setup is illustrated in Fig. 1. The velocity of the target plate is measured on the bottom surface. The target plate has dimensions of 3.5 cm by 0.45 cm, with vertical gaps positioned at $x = 1.25$ and $x = 3.25$, creating three distinct blocks. The gaps are placed to match experiments, with the center block being the target section of interest. All three pieces of the target plate are initially at rest. In this setup, the material of interest does not fill up the entire computational domain, which is a feature of using material point methods. The empty cells provide room for expected large material displacements or deformations. The use of empty cells requires only slight computational cost compared to filled ones, as most of the cost in the DDMP method is in the evaluation of the material points.

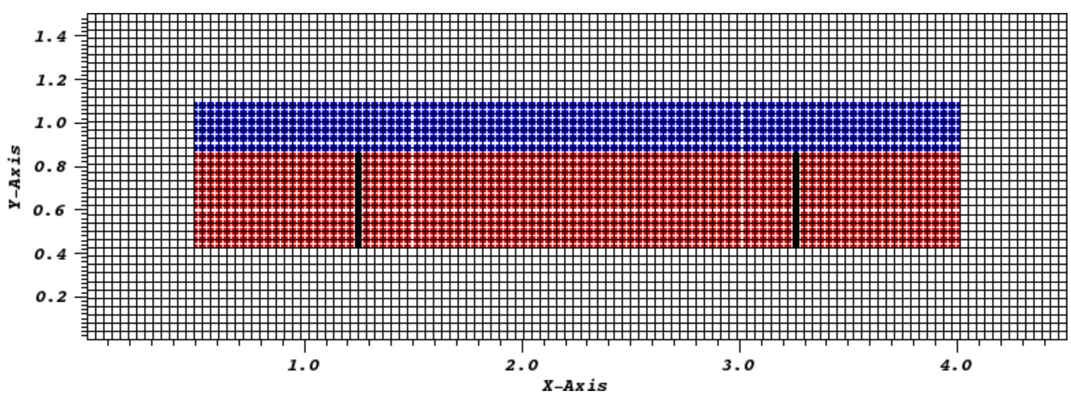

Figure 1: Plot of initial grid and particle positions. Blue indicates a flyer plate particle, and red is a test plate particle. Black vertical lines indicate crack locations.

Initially, the porosity of all three target plates is assumed to be at the minimum, $\Phi = 3.0 \times 10^{-4}$ as suggested in [7]. If the porosity falls below this value, we reset it to this value and treat any plastic flow at this level as classic plastic flow under the Johnson-Cook model.

Impact occurs at $t = 0$, and the simulation is run for 7 μs of physical time. Adaptive time stepping is utilized to ensure the CFL conditions are met on any given time step. All simulations are run serially, taking anywhere from 1 hour to two days to compute, depending on mesh resolution.

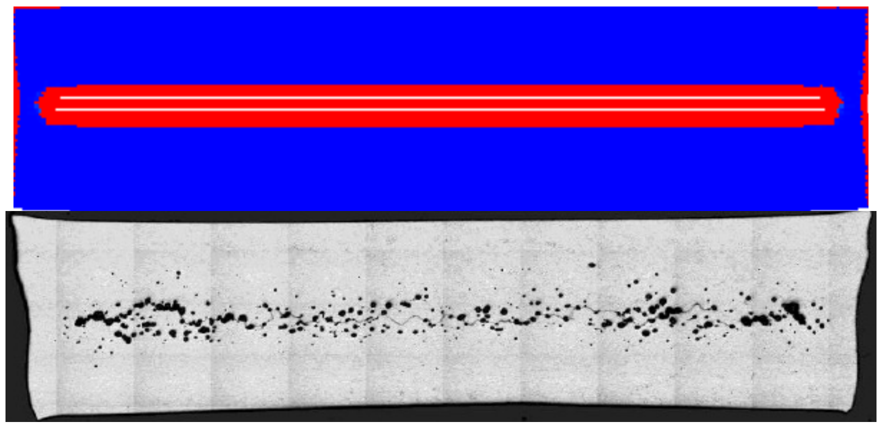

Figure 2: Plot of numerical porosity results (top) and experimental image (bottom). Numerical porosity is plotted, where blue is low porosity ($\Phi < 0.001$) and red is high porosity ($\Phi = 0.4$).

For a critical value of initial velocity of the flyer plate, voids are created in a typical ductile material leading to softening and eventually failure along the center line of the target plate as shown in Fig.2. The simulation was run using an underlying regular grid spacing of 150 μm.

The comparison of the calculated and measured target plate velocities on the bottom surface is shown in Fig. 3. Figure 4 shows results obtained using difference grid sizes. It shows overall converges under mesh refinement.

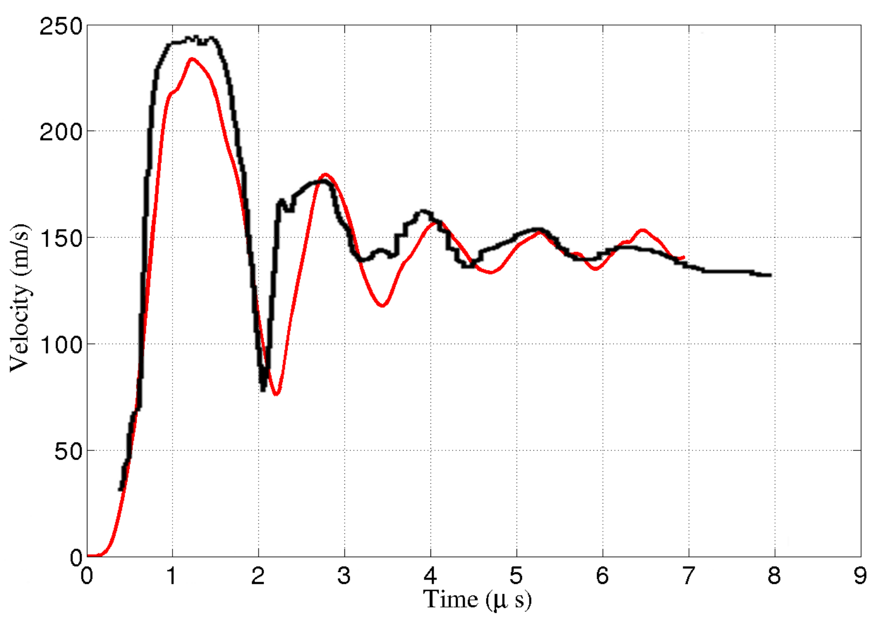

Figure 3: Plot of flyer plate velocity from both experimental (black) and numerical (red) results.

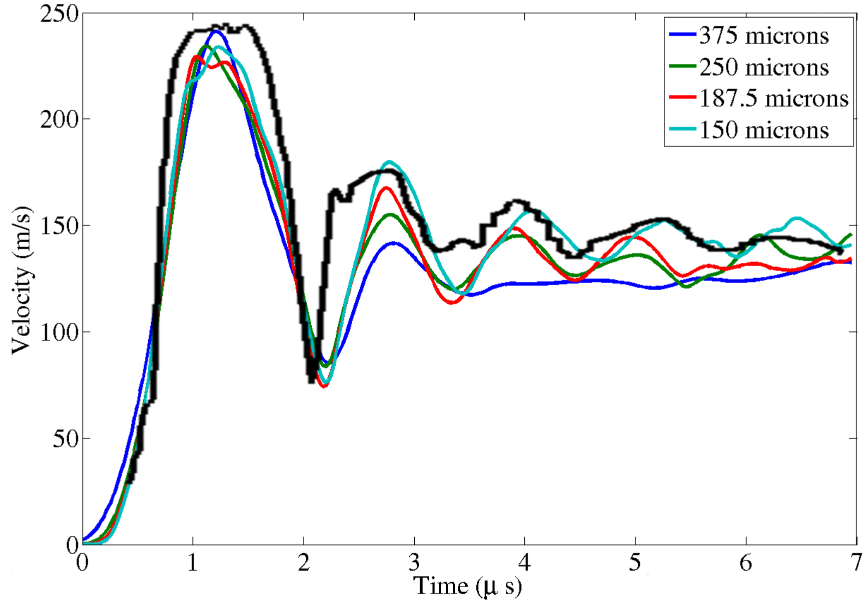

Figure 4: Plot of numerical flyer plate velocity with time. Simulations are presented using different mesh resolutions, with experimental results in black.

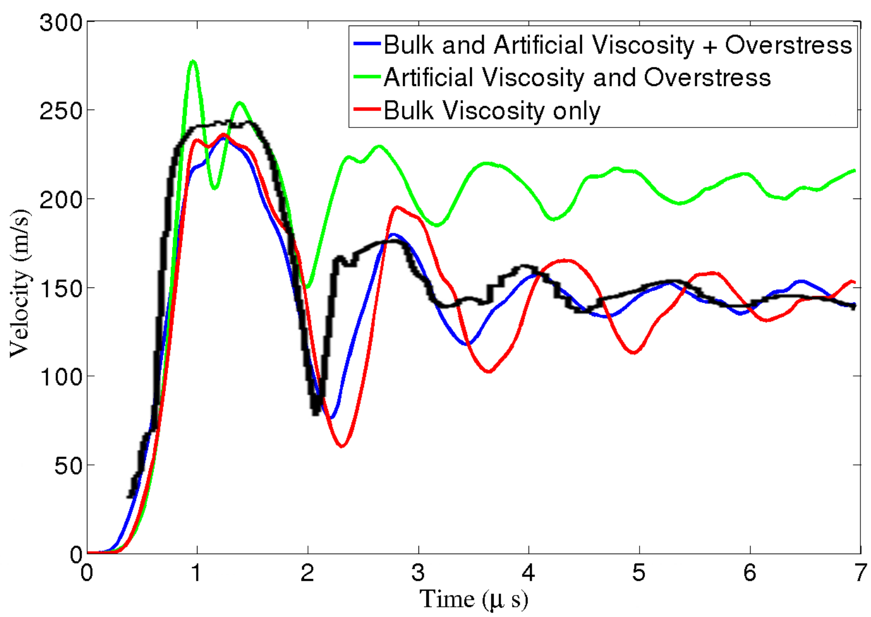

Figure 5: Comparison of Flyer plate velocity calculated with and without bulk viscosity. The green line is obtained without the bulk viscosity. The red line is obtained with bulk viscosity only. The blue line is obtained with overstress model and both bulk and artificial viscosities. Experimental results are shown in black for comparison.

Artificial viscosity has long been used to provide dissipation to noise near discontinuities in numerical systems. In our study, we find artificial viscosity is not necessary for this calculation, while physical bulk viscosity is essential as shown in Fig. 5. This figure also shows the overstress is also important for this problem of high strain rate.

Our choice of DDMP in these simulations is predicated on the fact that the material points will move out of their initial cells in the flyer plate simulation. It is expected that the numerical noise will be a significant issue, if only the MPM method is used. To confirm this and demonstrate the improvements brought about by DDMP, a simulation was run using traditional MPM, with the same physical and numerical parameters.

The velocity of the target plate with time is compared to the DDMP result and the experiment in Fig. 6. As can be seen, the velocity difference between the two methods is significant. A stress plot is also shown for each case in Fig. 7. The figure shows the stress field at 1.3 μs after the impact, when the stress field is critical to accurately project damage to the material. The MPM case demonstrates a large amount of "checkerboarding" in the stress field, which is caused by particles moving across cell boundaries, switching the signs on the internal forces. The DDMP method is clearly a dramatic improvement over the MPM in this regard.

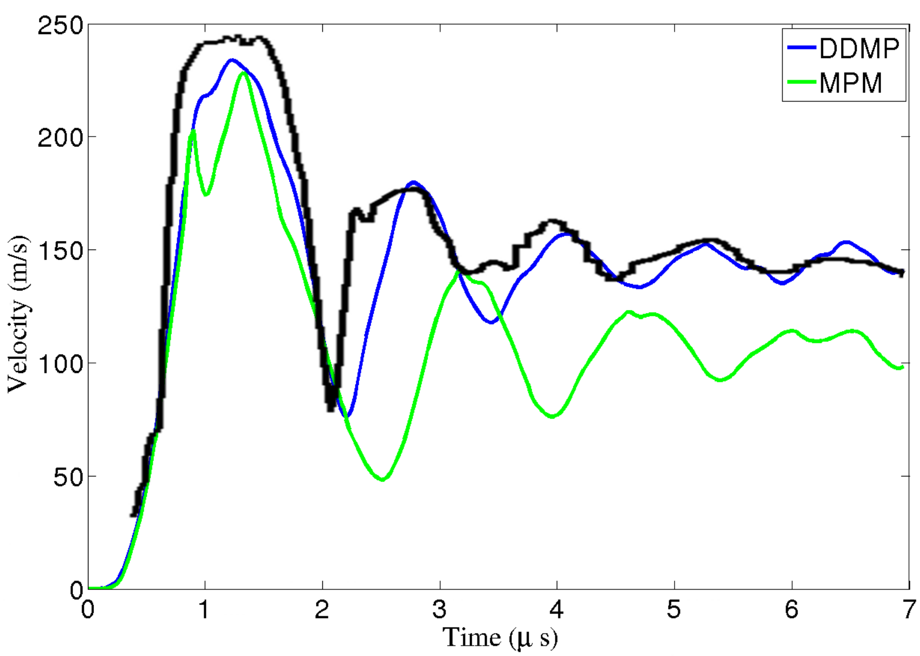

Figure 6: Target plate velocity of simulations run using MPM and DDMP. Experimental data shown in black.

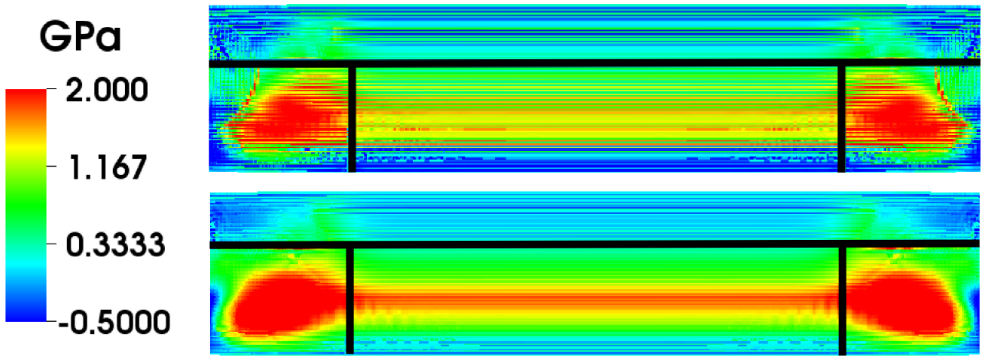

Figure 7: Stress field of σ_{yy} from MPM (top) and DDMP (bottom) at 1.3 μs.

3 Integrated Weapon Systems Modeling

To accelerate our effort on developing the coupled modeling capabilities, parallel to the TEPLA model implementation, we set up and performed can penetration simulations using the Johnson-Cook model without considering void growth. Figure 8 shows an axial symmetric penetration simulation of an aluminum can containing PBX 9501. The can has an inner diameter 11.43 cm, height 11.43 cm, and thickness 0.32 cm. The projectile is a steel ball of 1.27 cm in diameter. The initial projectile velocity is 1.882 km/s.

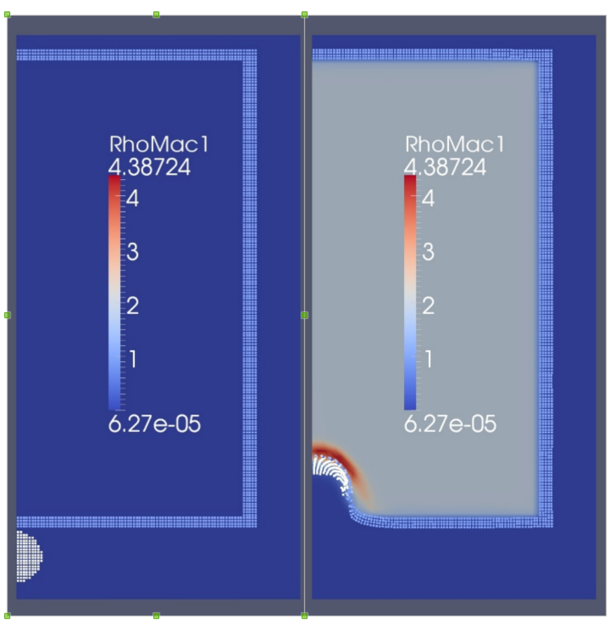

Figure 8: Numerical calculations of the can experiment.

As a comparison, a simulation of the same can experiment with a concave projectile of equal mass and diameter is also performed. Figure 9 shows distribution of the pressure and internal energy, which is proportional to the temperature, near the strike point 4 μs after the impact. The high pressure region is larger for the concave projectile. More importantly, the high pressure region is much closer to the high temperature region compared to the results for spherical projectile. The peak pressure is also higher in the cases of the concave projectile.

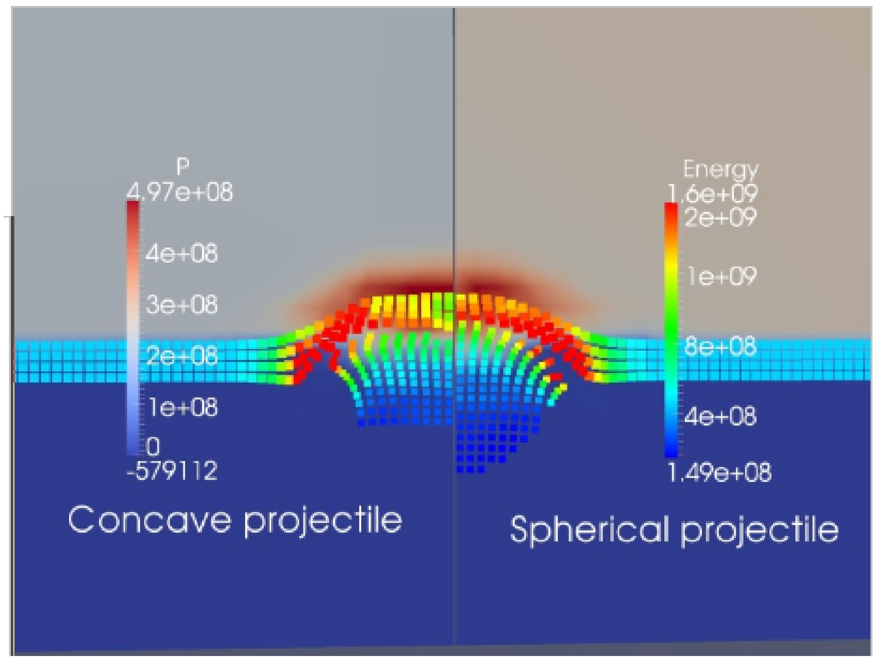

Figure 9: Pressure and internal energy distribution near the strike point 4 μs after the impact.

To better consider shock to detonation transition (SDT), SURF model with the JWL equation of state is also investigated. Currently, we have compared one-dimensional SDT waves with experiments as shown in Fig. 10

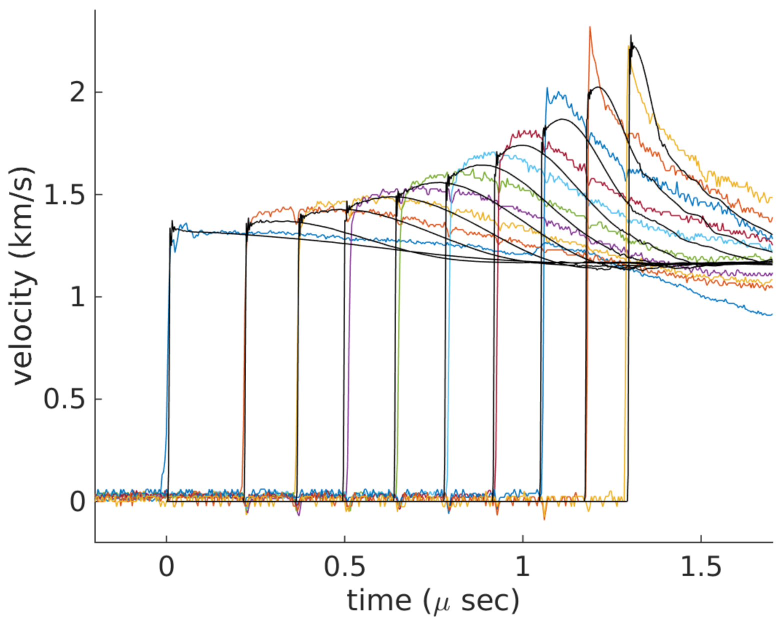

Figure 10: Comparison with 1-D SDT experiment. The smooth black-lines are from simulation, and the colored lines are experimental data.

4 Summary and Future Work

We implemented the TEPLA model for ductile damage and failure into the dual domain material point (DDMP) method framework. Simulations of a flyer plate problem are carried out using this implementation, and are compared with experimental measurements. While a traditional MPM approach fails due to excessive noise, DDMP performs quite well. These results further establish DDMP as a robust, viable method when dealing with problems involving strong history dependence and large material displacement. Further, the material model integrated with this material point approach was shown to perform in a stable fashion.

By studying the effects of artificial and bulk physical viscosities to the solution, we find that artificial viscosity is not necessary in this problem, while bulk physical viscosity is critical. The physical shear viscosity does not significantly affect the results either because the plastic flow provides sufficient energy dissipation for deviatoric deformation, while the bulk viscosity is the only energy dissipation mechanism for volumetric deformation in the current model. The relationship between high strain rate and the physical viscosity is a subject worth exploring in the future.

The implementation of the traditional version of the TEPLA model is in its final stages and will be applied to both penetration problems as well as other problems involving dynamic loading of materials. The model which has been developed over a number of years is one based upon small strain measures of deformation. In the next stages of work, this model will be extended to a large strain formulation which will allow for more accurate representation of material response for large deformation penetration problems and more consistent with general material modeling practices for finite strains. Implementation of SURF and JWL model capabilities will continue from the 1D testbed code to the full 3D implementation into CartaBlanca. This will require a number of validation steps to make sure the 3D implementation is consistent with that of the 1D testbed implementation. Completion of these implementations and verifying their stability and accuracy in CartaBlanca will the primary activity within FY16. Once this is completed we will begin to interact with the experimental community to seek our appropriate experiments to perform for validating the implementation and models, both on metallic materials as well as high explosives.

5 Acknowledgments

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